

Spin-spectral-weight distribution and energy range of the parent compound La_2CuO_4

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The spectral-weight distribution in recent neutron scattering experiments on the parent compound La_2CuO_4 (LCO), which are limited in energy range to about 450 meV, is studied in the framework of the Hubbard model on the square lattice. We find that the higher-energy weight extends to about 566 meV and is located at and near the momentum $[\pi, \pi]$. Our results confirm that the U/t value suitable to LCO is in the range $U/t \in (6, 8)$. The continuum weight energy-integrated intensity vanishes or is extremely small at momentum $[\pi, 0]$. This behavior of the intensity is consistent with that of spin waves, which are damped at $[\pi, 0]$.

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It is natural to expect that a greater understanding of the physics of the high- T_c superconductor undoped parent compounds, such as La_2CuO_4 (LCO), will lead to a greater understanding of the corresponding superconductors. In particular, the less complicated undoped systems can provide valuable information on which model Hamiltonians quantitatively describe the cuprates. Improved determination of the model Hamiltonians is essential because of the many nearby competing phases in the doped systems, easily affected by small parameters, which can now be seen because of continued improvements in numerical simulations [1]. A decade ago the neutron scattering experiments on LCO of Coldea, et. al. [2] first showed sufficient details of the spin-wave spectrum to demonstrate that a simple nearest-neighbor Heisenberg model must be supplemented by a number of additional terms, including ring exchanges. These terms arise naturally out of a single band Hubbard model with finite U/t , and several detailed studies showed that the spin-wave data in the available energy window could be successfully described by the Hubbard model using a somewhat smaller value of $U/t \sim 6 - 8$ than originally thought appropriate [2–5]. However, part of the spectral weight was deduced to be outside the energy window.

Recently, improved neutron scattering experiments [6] with a much wider energy window of about 450 meV, have raised a number of questions. Surprisingly, these studies revealed that the high-energy spin waves are strongly damped near momentum $[\pi, 0]$ and merge into a momentum-dependent continuum. These results led the authors of Ref. [6] to conclude that “the ground state of La_2CuO_4 contains additional correlations not captured by the Néel-SWT [spin-wave theory] picture”. This raises the important question of whether the more detailed results can still be described in terms of a simple Hubbard model. Here we address this question using a combination of a number of theoretical and numerical ap-

proaches, including, in addition to standard treatments, a new spinon approach for the spin excitations [5, 7] and density matrix renormalization group (DMRG) calculations for Hubbard cylinders [8–10]. We show that the Hubbard model *does* describe the new neutron scattering results. In particular, at momentum $[\pi, 0]$ the continuum weight energy-integrated intensity is found to vanish or be extremely small. Furthermore, we find that beyond 450 meV, the spectral weight is mostly located around momentum $[\pi, \pi]$ and extends to about 566 meV, suggesting directions for future experiments.

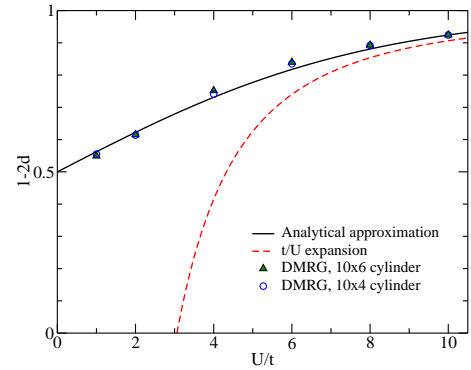


FIG. 1: Average single-occupancy: approximate expression $[1 + \tanh(U/8t)]/2$ valid for $U/t \leq 8$ (full line), the limiting $U/t \gg 1$ expression $[1 - c_0(8t/U)^2]$ (dashed line), and from DMRG numerical results on two different width cylinders.

The Hubbard model on a square lattice with $N \gg 1$ sites and periodic boundary conditions reads $\hat{H} = \hat{T} + U\hat{D}$. Here $\hat{T} = -t \sum_{\langle j, j' \rangle} \sum_{\sigma=\downarrow, \uparrow} [c_{\mathbf{r}_j, \sigma}^\dagger c_{\mathbf{r}_{j'}, \sigma} + h.c.]$ is the kinetic-energy operator, $\hat{D} = \sum_{j=1}^N \hat{n}_{\mathbf{r}_j, \uparrow} \hat{n}_{\mathbf{r}_j, \downarrow}$ counts the number of electron doubly occupied sites, $c_{\mathbf{r}_j, \sigma}^\dagger$ and $c_{\mathbf{r}_j, \sigma}$ are electron creation and annihilation operators with site index $j = 1, \dots, N$ and spin $\sigma = \uparrow, \downarrow$, and

$\hat{n}_{\mathbf{r}_j, \sigma} = c_{\mathbf{r}_j, \sigma}^\dagger c_{\mathbf{r}_j, \sigma}$. The expectation values,

$$d = \langle \hat{n}_{\mathbf{r}_j, \uparrow} \hat{n}_{\mathbf{r}_j, \downarrow} \rangle, \quad (1 - 2d) = \langle (\hat{n}_{\mathbf{r}_j, \uparrow} - \hat{n}_{\mathbf{r}_j, \downarrow})^2 \rangle, \\ m_{AF} = \frac{1}{2} \langle (-1)^j (\hat{n}_{\mathbf{r}_j, \uparrow} - \hat{n}_{\mathbf{r}_j, \downarrow}) \rangle \approx [1 - 2\delta S] m_{AF}^0, \quad (1)$$

play an important role in our study, following the strong evidence that for $U > 0$ and $N \rightarrow \infty$ the model ground state has antiferromagnetic long-range order [11]. In the last expression of Eq. (1), m_{AF}^0 stands for a mean-field sublattice magnetization that does not account for the effect of transverse fluctuations and δS accounts for such an effect, its value being estimated below. Moreover, $\hat{S}_{\mathbf{r}_j}^z = \frac{1}{2}[\hat{n}_{\mathbf{r}_j, \uparrow} - \hat{n}_{\mathbf{r}_j, \downarrow}]$, $\hat{S}_{\mathbf{r}_j}^x = \frac{1}{2}[\hat{S}_{\mathbf{r}_j}^+ + \hat{S}_{\mathbf{r}_j}^-]$, $\hat{S}_{\mathbf{r}_j}^y = \frac{1}{2i}[\hat{S}_{\mathbf{r}_j}^+ - \hat{S}_{\mathbf{r}_j}^-]$, $\hat{S}_{\mathbf{r}_j}^+ = c_{\mathbf{r}_j, \uparrow}^\dagger c_{\mathbf{r}_j, \downarrow}$, and $\hat{S}_{\mathbf{r}_j}^- = c_{\mathbf{r}_j, \downarrow}^\dagger c_{\mathbf{r}_j, \uparrow}$. Our study involves the dynamical structure factors,

$$S^{\alpha\alpha'}(\mathbf{k}, \omega) = \frac{(g\mu_B)^2}{N} \sum_{j, j'=1}^N e^{-i\mathbf{k}(\mathbf{r}_j - \mathbf{r}_{j'})} \\ \times \int_{-\infty}^{\infty} dt e^{i\omega t} \langle GS | \hat{S}_{\mathbf{r}_j}^\alpha(t) \hat{S}_{\mathbf{r}_{j'}}^{\alpha'}(0) | GS \rangle, \quad (2)$$

where $\alpha = \alpha' = x, y, z$ or $\alpha = -$ and $\alpha' = +$ and below we consider $g = 2$. It is straightforward to show that the sum rules $[1/N] \sum_{\mathbf{k}} S^{\alpha\alpha'}(\mathbf{k})$ where $S^{\alpha\alpha'}(\mathbf{k}) = [1/2\pi] \int_{-\infty}^{\infty} d\omega S^{\alpha\alpha'}(\mathbf{k}, \omega)$ involve the average single occupancy $(1 - 2d)$ and read $[(g\mu_B)^2/4][\delta_{\alpha, \alpha'} + 2\delta_{\alpha, -} \delta_{\alpha', +}](1 - 2d)$. In an ideal experiment one sees a transfer of weight from the longitudinal to the transverse part such that independent of the scattering geometry, the corresponding effective spin form factor satisfies the sum rule,

$$\frac{1}{N} \sum_{\mathbf{k}} \frac{1}{2\pi} \int_{-\infty}^{\infty} d\omega S^{exp}(\mathbf{k}, \omega) = \mu_B^2 2(1 - 2d). \quad (3)$$

That the coefficient involved is $2(1 - 2d)$ rather than $3(1 - 2d)$ follows from in the experiment one mode being perpendicular to the plane and thus silent [4].

For $U/t \in (0, 8)$ the antiferromagnetic long-range order may be accounted for by a variational ground state with a SDW initial trial state, such as $|G\rangle = e^{-g\hat{D}}|SDW\rangle$ or $|GB\rangle = e^{-h\hat{T}/t} e^{-g\hat{D}}|SDW\rangle$, where $|SDW\rangle$ is the ground state of a simple effective mean-field Hamiltonian, as that of Eq. (18) of Ref. [12]. For $U/t \gg 1$ such an order is as well accounted for by a Baeriswyl variational state $|B\rangle = e^{-h\hat{T}/t}|\infty\rangle$ where $|\infty\rangle$ is the exact $U/t \rightarrow \infty$ ground state [12]. The coefficients h and g multiplying the kinetic-energy and double-occupancy operators, respectively, are variational parameters. Similarly for the trial state $|SDW\rangle$, the relation $4[m_{AF}^0]^2 = (1 - 4d)$ holds for $|G\rangle$, $|GB\rangle$, and $|B\rangle$, while the function $d = d(U/t)$ is state dependent. This gives $d = \frac{1}{4}[1 - 4[m_{AF}^0]^2]$, consistent with d not being affected by transverse fluctuations.

The evaluation of the ground-state energy for $|GB\rangle$ and $|B\rangle$ is for $N \gg 1$ an involved problem. Here we resort

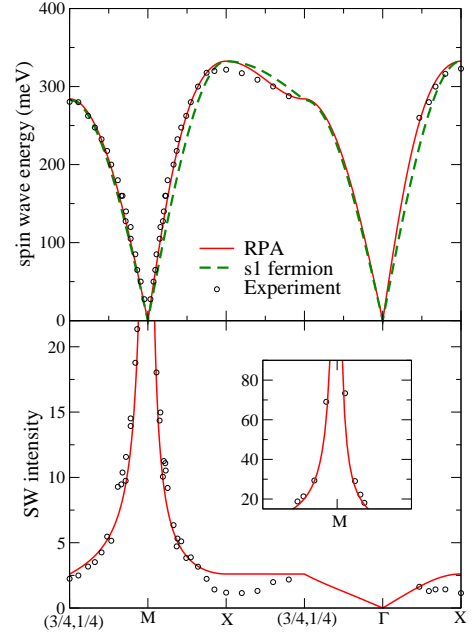


FIG. 2: Upper panel: Spin-wave excitation spectrum along Brillouin-zone special directions as specified in Ref. [6]. Lower panel: Spin-wave intensity as obtained from the poles of the susceptibility (see text). Experimental points from Ref. [6].

to an approximation, which corresponds to the simplest expression of the general form $E/N = T_0 q_U + Ud$ where $T_0 = -\frac{16}{\pi^2} t$ compatible with three requirements: the relation $d = \frac{1}{4}[1 - 4[m_{AF}^0]^2]$; the occurrence of antiferromagnetic long-range order for the whole $U/t > 0$ range; and the lack of a linear kinetic-energy term in U for $U/t \ll 1$. Brinkman and Rice found $q_U = 8d(1 - 2d)$ for the original Gutzwiller approximation [13], which is lattice insensitive and thus does not account for the square-lattice antiferromagnetic long-range order. The simplest modified form of the quantity q_U such that the three conditions are met is $q_U = \left(\frac{U}{8t}\right) a_1^{(+)} d \left[\frac{(1-2d)}{4[m_{AF}^0]^2} - a_2 \right] - a_3$ where $4[m_{AF}^0]^2$ behaves as $4[m_{AF}^0]^2 = U/8t$ for $U/t \ll 1$, $a_1^{(\pm)} = \pi^2 \pm 4$, $a_2 = (1 - [\pi^2/2a_1^{(+)}])$, and $a_3 = a_3(U/8t)$ a function given by $a_3 = [a_1^{(-)}/8]\{1 - \tanh([U/8t][(4 + a_1^{(+)})/a_1^{(-)}])\}$ for $U/t \in (0, 8)$ and $a_3 = -c_0[\pi/2]^2 [8t/U]$ for $U/t \gg 1$. Here $c_0 = [\alpha/4 + 1/8]/2 = 0.1462$ and the corresponding estimate $\alpha = 0.6696$ is that of the Heisenberg-model studies of Ref. [11]. Minimization of the obtained ground-state energy with respect to d leads indeed to $d = \frac{1}{4}[1 - 4[m_{AF}^0]^2]$. For $U/t \ll 1$ such a q_U expression yields to second order in U/t , $E/N = T_0 + Ud - [1/8\pi^2][U^2/t]$ where $[1/8\pi^2] \approx 0.0127$. The coefficient ≈ -0.0127 is that also obtained by second-order perturbation theory [14]. For $U/t \gg 1$ one recovers the known result $E/N = -4c_0[8t^2/U]$ [11], so that our approximation agrees with the known limiting behaviors.

For $U/t \in (0, 8)$, we find that $4[m_{AF}^0]^2 \approx \tanh(U/8t)$ gives quantitative agreement for the $(1-2d)$ dependence on U/t with both our numerical DMRG calculations (see Fig. 1) and the numerical results for the states $|G\rangle$ and $|GB\rangle$ (see Fig. 4 of Ref. [4]). In the DMRG calculations, two different circumference cylinders were simulated as a function U/t , with open boundary conditions in x and periodic in y , and the double occupancy measured in one of the middle columns. A maximum of $m = 4000$ states were kept, with an accuracy of $\sim 10^{-4}$ in $(1-2d)$ for the 10×4 system for the least accurate smaller U/t values, and about 10^{-3} for the 10×6 system. We find that the value of $(1-2d)$ is relatively insensitive to cluster size, and these cluster sizes are representative of 2D behavior [15]. For $U/t \gg 1$ we find the behavior $4[m_{AF}^0]^2 \approx e^{-2c_0(8t/U)^2}$ for the state $|B\rangle$, so that $(1-2d) = [1 + \tanh(U/8t)]/2$ for approximately $U/t \leq 8$ and $(1-2d) = [1 - c_0(8t/U)^2]$ for $U/t \gg 1$. Furthermore, the states $|SDW\rangle$ and $|B\rangle$ give $m_{AF} \approx m_{AF}^0 = \frac{1}{2}\sqrt{1-4d}$, with an improved $d = d(U/t)$ dependence for the latter, whose m_{AF}^0 magnitudes are provided below in Table I for several U/t values. The states $|GB\rangle$ and $|B\rangle$ have m_{AF}^{GB} and m_{AF}^B sublattice magnetization numerical values very close to those given by Eq. (1) with $\delta S \approx d$ and $\delta S \approx d + \frac{1}{2}[1 - m_{HAF}/m_{HAF}^0] \approx d + 0.197$, respectively. Here $m_{HAF}^0 = 1/2$ and $m_{HAF} \approx 0.303$ is the Heisenberg-model sublattice magnetization magnitude [11]. Some m_{AF}^{GB} magnitudes are given below in Table I, along with those of $m_{AF}^{lower} = (1-2d)[m_{HAF}/m_{HAF}^0]m_{AF}^0$, which we define for $U/t > 0$ and for $U/t \gg 1$ becomes m_{AF}^B . Probably m_{AF}^{lower} is closest to the exact m_{AF} , while m_{AF}^{GB} is consistent with our use of the RPA.

To study the coherent spin-wave weight distribution and spectrum, we have calculated by RPA the transverse dynamical susceptibility $\chi^{-+}(\mathbf{k}, \tau) = \frac{(g\mu_B)^2}{N} \sum_{j,j'=1}^N e^{-i\mathbf{k}\cdot(\mathbf{r}_j-\mathbf{r}_{j'})} \langle \hat{S}^-(\mathbf{r}_j, \tau) \hat{S}^+(\mathbf{r}_{j'}, 0) \rangle$, where τ denotes the imaginary time in Matsubara formalism (we shall take the zero temperature limit). In the case of the present model, the coherent spin-wave spectral weight in units of μ_B^2 is $Z_d 2(1-2d)$. Here $Z_d = 1 - [2/N(1-2d)] \sum_{\mathbf{k}} \sum_{\nu' \neq \nu} |\langle \nu' | \hat{S}_{\mathbf{k}}^+ | GS \rangle|^2$ where the sum over energy eigenstates excludes those that generate the coherent spin-wave weight, $|\nu\rangle = |\nu, \omega(\mathbf{k})\rangle$. In the $U/t \rightarrow \infty$ limit, Z_d may be identified with the corresponding $Z_d = Z_c Z_\chi$ factor of the Heisenberg model on the square lattice. According to the results of Ref. [16], $Z_c \approx 1.18$ and $Z_\chi \approx 0.48$, respectively, so that $Z_d \approx 0.57$. The limiting values $Z_d = 1$ for $U/t \rightarrow 0$ and $Z_d \approx 0.57$ for $U/t \rightarrow \infty$ and the approximate intermediate value $Z_d \approx 0.65$ at $U/t = 8$ [4] are recovered as solutions of the equation $Z_d = e^{-Z_d \tanh(\sqrt{\frac{U}{4\pi t}})}$, which is used here for finite U/t . In the thermodynamic limit the upper-Hubbard band processes generate nearly no spin weight. Hence the longitudinal (elastic contribution to) spectral weight within $\mu_B^2 2(1-2d)$, Eq. (3), is in units of μ_B^2

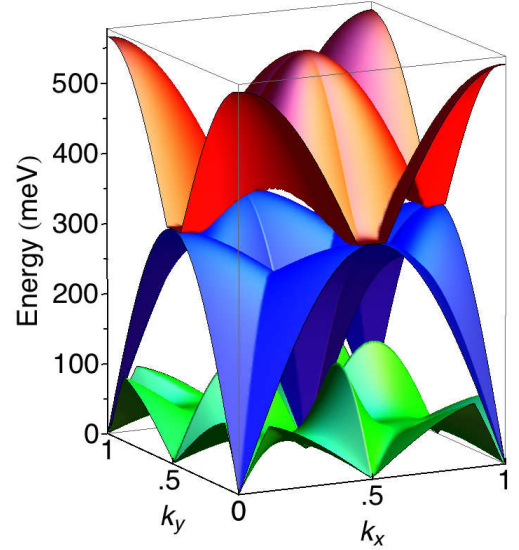


FIG. 3: The energy-momentum space limits of the spin $S = 1$ excited states spectrum for $U/t = 6.1$, $t = 295$ meV, and k_x and k_y in units of 2π . States whose energy is for a given \mathbf{k} lower than that of the intermediate spin-wave sheet as well as those of any energy and equivalent momenta $[0, 0] = [0, 2\pi] = [2\pi, 0] = [2\pi, 2\pi]$ do not contribute to the spin spectral weight.

approximately given by $\approx 4(m_{AF})^2$ and the spin-wave intensity reads $W_{SW} = Z_d [2(1-2d) - 4(m_{AF})^2]$. The GA+RPA method used in Ref. [4] accounts for the quantum fluctuations that control the longitudinal and transverse relative weights, so that the spin-wave intensity factor is Z_d . The RPA used here leads to a similar spin-wave intensity momentum distribution but its experimentally determined factor $Z_d^{exp} < Z_d$ is such that $W_{SW} = Z_d [2(1-2d) - 4(m_{AF})^2] = Z_d^{exp} 2(1-2d)$.

Within the two-sublattice description the susceptibility becomes a 2×2 tensor and the above original susceptibility $\chi^{-+}(\mathbf{k}, \tau)$ is the average of its four elements. After Fourier transforming to $(\mathbf{k}, i\omega)$ space, within the RPA the susceptibility tensor obeys $\tilde{\chi}^{RPA} = [1 - U\tilde{\chi}^{(0)}]^{-1} \tilde{\chi}^{(0)}$. Here $\tilde{\chi}^{(0)}$ denotes the susceptibility tensor in the noninteracting system. $\tilde{\chi}^{RPA}$ has a pole $i\omega = \omega(\mathbf{k})$ obtained from the equation $\text{Det}[1 - U\tilde{\chi}^{(0)}] = 0$, which provides the dispersion relation $\omega(\mathbf{k})$ for the spin waves. It has been shown in Ref. [3] that an excellent agreement with the spin-wave spectrum from Ref. [2] is achieved. In Fig. 2 upper panel we show a fit to the more recent experimental data of Ref. [6] (full line) along with the results from the $s1$ fermion method reported below (dotted line) for $U/t = 6.1$ and $t = 295$ meV. Provided that the t magnitude is slightly increased for increasing values of U/t , agreement with the LCO spin-weight spectrum and distribution can be obtained for $U/t \in (6, 8)$. For U/t values smaller than 6 (and larger than 8), the spin-wave dispersion between $[\pi/2, 0]$ and $[\pi/2, \pi/2]$ has a too large

energy bandwidth (and is too flat) for any reasonable value of t . From the residue of the spin-wave pole the susceptibility coherent part reads,

$$\chi_{co}^{-+}(\mathbf{k}, i\omega) = Z_d^{exp} \sum_{l=\pm 1} \frac{\text{Res}[\chi^{-+}(\mathbf{k}, l\omega(\mathbf{k}))]}{i\omega - l\omega(\mathbf{k})}. \quad (4)$$

The measured intensity is $I_{SW}(\mathbf{k}) = \pi[S^{xx}(\mathbf{k}) + S^{yy}(\mathbf{k})] = \pi S^{-+}(\mathbf{k})$ [17]. In Fig. 2 lower panel, we plot the corresponding RPA spin-wave intensity, $I_{SW}(\mathbf{k}) = -[\pi/2]Z_d^{exp}\text{Res}[\chi^{-+}(\mathbf{k}, \omega(\mathbf{k}))]$. The good agreement with the experimental data, specially near the point M , reproduces the theoretical results of Ref. [6]. It is here obtained for the value $Z_d^{exp} \approx 0.49$, which corresponds to the choice $m_{AF} = m_{AF}^{GB} = m_{AF}^0(1 - 2d)$ such that $\delta S \approx d$. As in Ref. [6], it shows disagreement around the X point, which here probably stems from the RPA.

To derive the spectrum of the spin $S = 1$ excited states producing the inelastic form-factor spectral weight, we use the spinon operator representation of Ref. [5]. The ground-state spin degrees of freedom are described by a full $s1$ fermion band, which coincides with an antiferromagnetic reduced Brillouin zone. Each $s1$ fermion is a spin-singlet two-spinon composite object. The spin $S = 1$ excited states of momentum $\mathbf{k} = [\pi, \pi] - \mathbf{q} - \mathbf{q}'$ are generated upon breaking one $s1$ fermion spinon pair, which leads to the emergence of two holes of momenta \mathbf{q} and \mathbf{q}' in the otherwise full $s1$ band. The inelastic coherent spin-wave spectrum is generated by processes where \mathbf{q} points in the nodal direction and \mathbf{q}' belongs to the boundary of the $s1$ band reduced zone [5]. The remaining choices of \mathbf{q} and \mathbf{q}' either generate the inelastic incoherent continuum spectral weight or vanishing weight, respectively. The studies of Ref. [5] are limited to the spin-wave spectrum. Here we consider the energy-momentum space domain of all above spin $S = 1$ excited states, which is represented in Fig. 3. (A similar spectrum is obtained for the values $U/t = 8.0$ and $t = 335$ meV of Ref. [4].) The intermediate sheet refers to the spin-wave spectrum. For each \mathbf{k} , states of energy lower than the latter spectrum do not contribute to the form-factor weigh. Furthermore and consistent with the first-moment sum rules of an isotropic antiferromagnet, no and nearly no weight is generated by states of any energy and momentum $[0, 0]$ and near $[0, 0]$, respectively. Unfortunately, the method of Ref. [5] does not provide the detailed continuum weight distribution. However, it is expected that, similarly to the Heisenberg model case [4], its energy-integrated intensity follows the same trend as the spin-wave intensity. Analysis of Fig. 3 reveals that for momentum $[\pi, 0]$ there are no excited states of energy higher than the spin waves. Thus at momentum $[\pi, 0]$, the continuum weight distribution energy-integrated intensity vanishes or is extremely small, due to $s1$ band four-hole processes. Given the expected common trend of both intensities, this is consistent with a damping of

U/t	6.1	6.5	8.0	10.0
W_T	1.643	1.671	1.762 (1.778 [4])	1.848 (1.846 [4])
W_{SW}	0.808	0.799	0.761	0.714
$W_{<450}$	1.571	1.593	1.663	1.730
$W_{>450}$	0.072	0.078	0.099	0.118
m_{AF}^0	0.401	0.410	0.436 (0.43 [4, 12])	0.461 (0.456 [4])
m_{AF}^{GB}	0.329	0.342	0.384 (0.39 [12])	0.426
m_{AF}^{lower}	0.200	0.207	0.233	0.258

TABLE I: Several spectral weights in units of μ_B^2 as defined in the text and the sublattice magnetizations as calculated here for several U/t values and some results from Refs. [4, 12].

the spin-wave intensity at momentum $[\pi, 0]$, as observed [6] but not captured by the Fig. 2 RPA intensity.

In Table I we provide the sublattice magnetization magnitudes along with our calculations of the following integrated spectral weights (in units of μ_B^2): the total weight, $W_T = 2(1 - 2d)$; the spin-wave weight, $W_{SW} = Z_d^{exp} 2(1 - 2d)$; the weight for energy $\hbar\omega \leq 450$ meV, $W_{<450} = W_{SW}/0.71 + 4(m_{AF}^{GB})^2$; and the weight $W_{>450} = [W_T - W_{<450}]$ for energy $\hbar\omega > 450$ meV. $W_{<450}$ is derived by combining our theoretical expressions with the observations of Ref. [6] that for the energy range up to about 450 meV, 71% and 29% of the weight corresponding to the inelastic response comes from the coherent spin-wave weight and incoherent continuum weight, respectively. Our prediction for $W_{<450}$ varies between $1.6 \mu_B^2$ for $U/t \approx 6.1$ and $1.7 \mu_B^2$ for $U/t \approx 8.0$, in agreement with the experimental value $1.9 \pm 0.3 \mu_B^2$ reported in Ref. [6]. From our above analysis, the small weight $W_{>450} \approx 0.1 \mu_B^2$ is expected to extend to about 566 meV (see Fig. 3), mostly at and around the momentum $[\pi, \pi]$.

Our result that at momentum $[\pi, 0]$ the continuum weight energy-integrated intensity vanishes or is very small is consistent with a corresponding damping of the spin-wave intensity at $[\pi, 0]$, as observed in the recent experiments of Ref. [6]. We suggest that future LCO neutron scattering experiments scan the energies between 450 meV and 566 meV and momenta around $[\pi, \pi]$.

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